MPI for Scalable Computing (continued from yesterday)

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Topology Mapping and Neighborhood Collectives

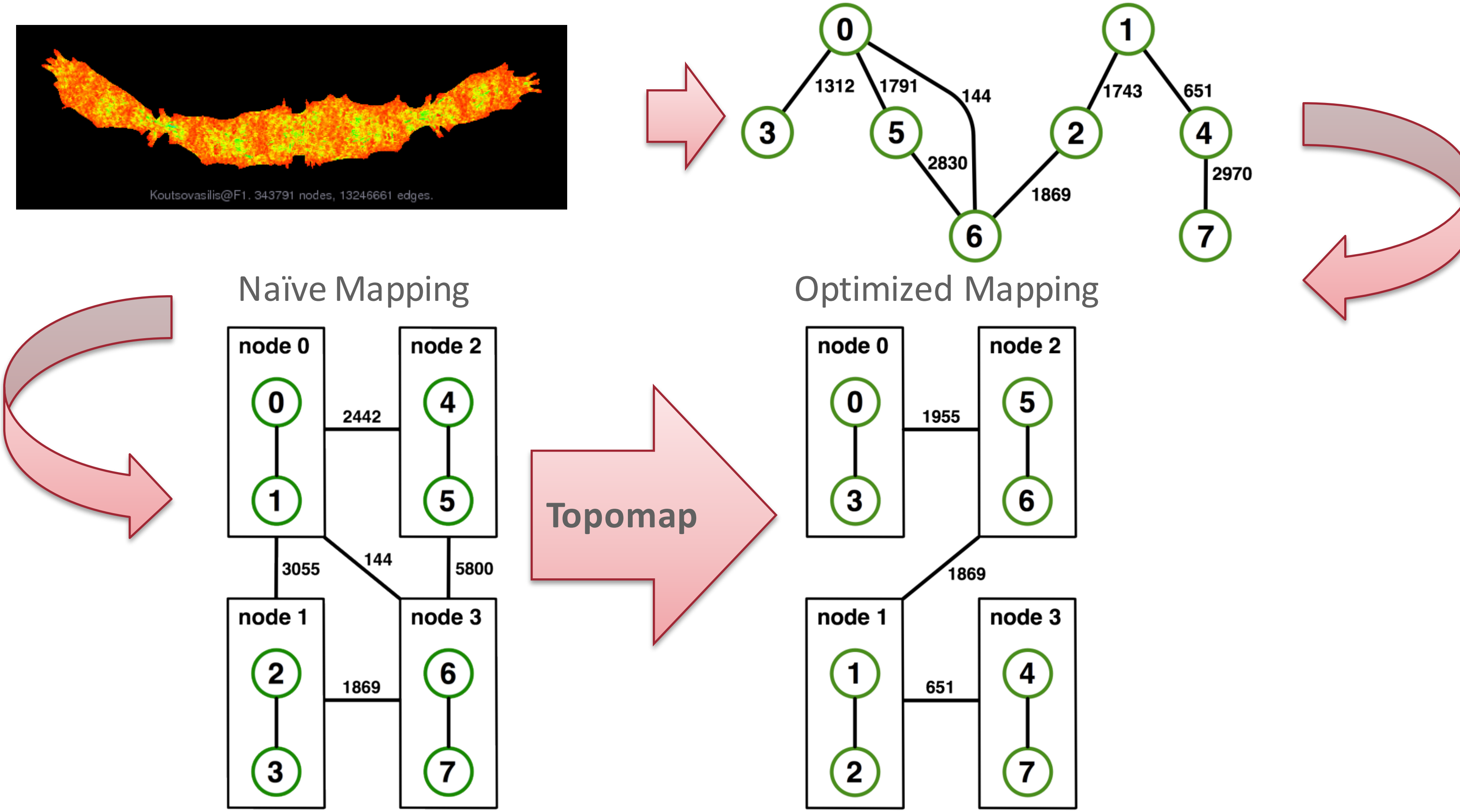
Topology Mapping Basics

- First type: Allocation mapping
  - Up-front specification of communication pattern
  - Batch system picks good set of nodes for given topology
- Properties:
  - Not widely supported by current batch systems
  - Either predefined allocation (BG/P), random allocation, or "global bandwidth maximation"
  - Also problematic to specify communication pattern upfront, not always possible (or static)

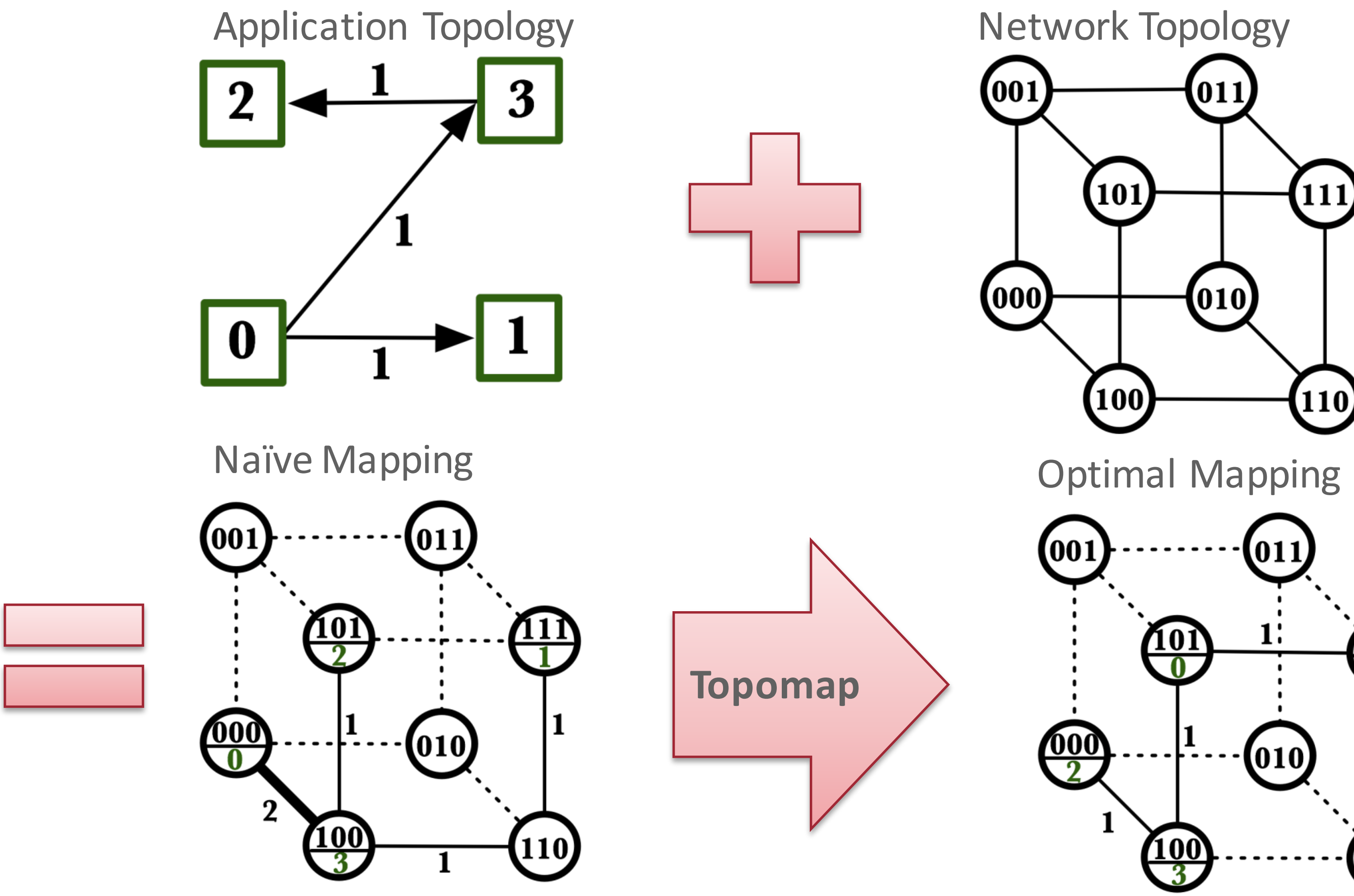
Topology Mapping Basics

- Rank reordering
  - Change numbering in a given allocation to reduce congestion or dilation
  - Sometimes automatic (early IBM SP machines)
- Properties
  - Always possible, but effect may be limited (e.g., in a bad allocation)
  - Portable way: MPI process topologies
    - Network topology is not exposed
  - Manual data shuffling after remapping step

On-Node Reordering



Off-Node (Network) Reordering



MPI Topology Intro

- Convenience functions (in MPI-1)
  - Create a graph and query it, nothing else
  - Useful especially for Cartesian topologies
    - Query neighbors in n-dimensional space
  - Graph topology: each rank specifies full graph ☹
- Scalable Graph topology (MPI-2.2)
  - Graph topology: each rank specifies its neighbors **or** an arbitrary subset of the graph
- Neighborhood collectives (MPI-3.0)
  - Adding communication functions defined on graph topologies (neighborhood of distance one)

MPI_Cart_create

```
MPI_Cart_create(MPI_Comm comm_old, int ndims,
        const int *dims, const int *periods, int reorder,
        MPI_Comm *comm_cart)
```

- Specify ndims-dimensional topology
  - Optionally periodic in each dimension (Torus)
- Some processes may return MPI_COMM_NULL
  - Product of dims must be ≤ P
- Reorder argument allows for topology mapping
  - Each calling process may have a new rank in the created communicator
  - Data has to be remapped manually

MPI_Cart_create Example

```
int dims[3] = {5,5,5};
int periods[3] = {1,1,1};
MPI_Comm topocomm;
MPI_Cart_create(comm, 3, dims, periods, 0, &topocomm);
```

- But we're starting MPI processes with a one-dimensional argument (-p X)
  - User has to determine size of each dimension
  - Often as "square" as possible, MPI can help!

MPI_Dims_create

```
MPI_Dims_create(int nnodes, int ndims, int *dims)
```

- Create dims array for Cart_create with nnodes and ndims
  - Dimensions are as close as possible (well, in theory)
- Non-zero entries in dims will not be changed
  - nnodes must be multiple of all non-zeroes in dims

MPI_Dims_create Example

```
int p;
int dims[3] = {0,0,0};
MPI_Comm_size(MPI_COMM_WORLD, &p);
MPI_Dims_create(p, 3, dims);

int periods[3] = {1,1,1};
MPI_Comm topocomm;
MPI_Cart_create(comm, 3, dims, periods, 0, &topocomm);
```

- Makes life a little bit easier
  - Some problems may be better with a non-square layout though

Cartesian Query Functions

- Library support and convenience!
- MPI_Cartdim_get()
  - Gets dimensions of a Cartesian communicator
- MPI_Cart_get()
  - Gets size of dimensions
- MPI_Cart_rank()
  - Translate coordinates to rank
- MPI_Cart_coords()
  - Translate rank to coordinates

Cartesian Communication Helpers

```
MPI_Cart_shift(MPI_Comm comm, int direction, int disp,
int *rank_source, int *rank_dest)
```

- Shift in one dimension
  - Dimensions are numbered from 0 to ndims-1
  - Displacement indicates neighbor distance (-1, 1, …)
  - May return MPI_PROC_NULL
- Very convenient, all you need for nearest neighbor communication

MPI_Graph_create

- Don't use! Use one of the Dist_graph functions instead

```
MPI_Graph_create(MPI_Comm comm_old, int nnodes,
        const int *index, const int *edges, int reorder,
        MPI_Comm *comm_graph)
```

- nnodes is the total number of nodes
- index i stores the total number of neighbors for the first i nodes (sum)
  - Acts as offset into edges array
- edges stores the edge list for all processes
  - Edge list for process j starts at index[j] in edges
  - Process j has index[j+1]-index[j] edges

Distributed graph constructor

- MPI_Graph_create is discouraged
  - Not scalable
  - Not deprecated yet but hopefully soon
- New distributed interface:
  - Scalable, allows distributed graph specification
    - Either local neighbors **or** any edge in the graph
  - Specify edge weights
    - Meaning undefined but optimization opportunity for vendors!
  - Info arguments
    - Communicate assertions of semantics to the MPI library
    - E.g., semantics of edge weights

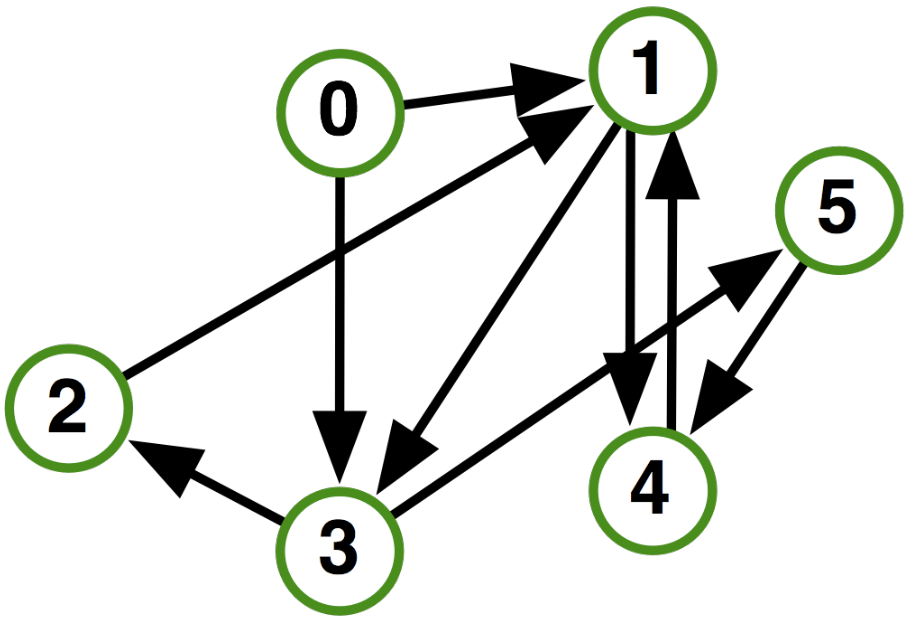
MPI_Dist_graph_create_adjacent

```
MPI_Dist_graph_create_adjacent(MPI_Comm comm_old, int indegree,
        const int sources[], const int sourceweights[], int outdegree,
        const int destinations[], const int destweights[],
        MPI_Info info, int reorder, MPI_Comm *comm_dist_graph)
```

- indegree, sources, sourceweights – source proc. spec.
- outdegree, destinations, destweights – dest. proc. spec.
- info, reorder, comm_dist_graph – as usual
- directed graph
- Each edge is specified twice, once as out-edge (at the source) and once as in-edge (at the dest)

MPI_Dist_graph_create_adjacent

- Process 0:
  - Indegree: 0
  - Outdegree: 2
  - Dests: {3,1}
- Process 1:
  - Indegree: 3
  - Outdegree: 2
  - Sources: {4,0,2}
  - Dests: {3,4}
- …



MPI_Dist_graph_create

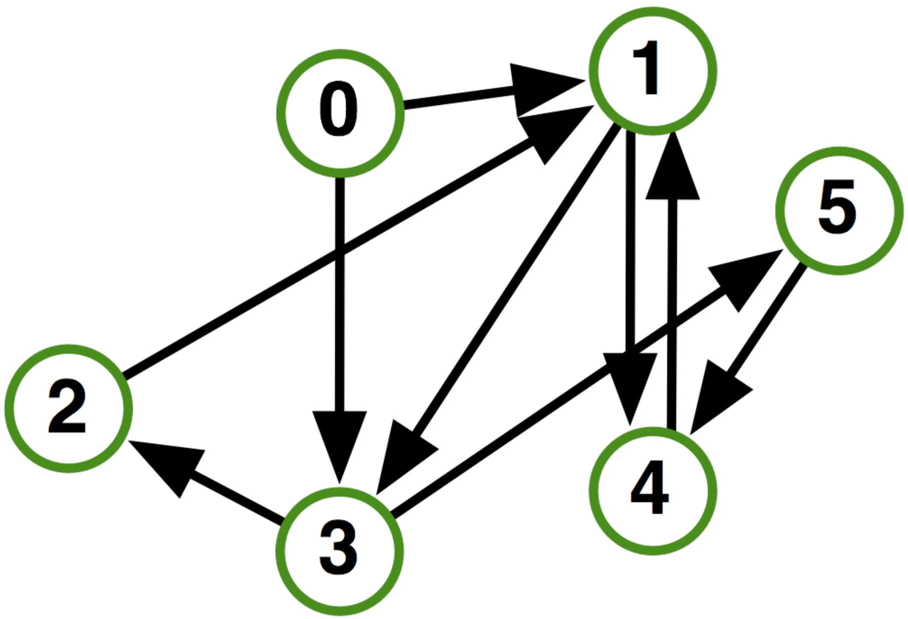
```
MPI_Dist_graph_create(MPI_Comm  comm_old, int n,
        const int sources[], const int degrees[],
        const int destinations[], const int weights[],
        MPI_Info info, int reorder,
        MPI_Comm *comm_dist_graph)
```

- n – number of source nodes
- sources – n source nodes
- degrees – number of edges for each source
- destinations, weights – dest. process specification
- info, reorder – as usual
- More flexible and convenient
  - Requires global communication
  - Slightly more expensive than adjacent specification

Hoefler et al.: The Scalable Process Topology Interface of MPI 2.2

MPI_Dist_graph_create

- Process 0:
  - N: 2
  - Sources: {0,1}
  - Degrees: {2,2}
  - Dests: {3,1,4,3}
- Process 1:
  - N: 2
  - Sources: {2,3}
  - Degrees: {1,1} *
  - Dests: {1,2}
- …



* Note that in this example, process 1 specifies only one of the two outgoing edges of process 3; the second outgoing edge needs to be specified by another process

Distributed Graph Neighbor Queries

- MPI_Dist_graph_neighbors_count()

```
MPI_Dist_graph_neighbors_count(MPI_Comm  comm,
        int *indegree,  int *outdegree,  int *weighted)
```

  - Query the number of neighbors of **calling process**
  - Returns indegree and outdegree!
  - Also info if weighted

- MPI_Dist_graph_neighbors()
  - Query the neighbor list of **calling process**
  - Optionally return weights

```
MPI_Dist_graph_neighbors(MPI_Comm  comm,
        int maxindegree,  int sources[], int sourceweights[],
        int maxoutdegree,  int destinations[],int destweights[])
```

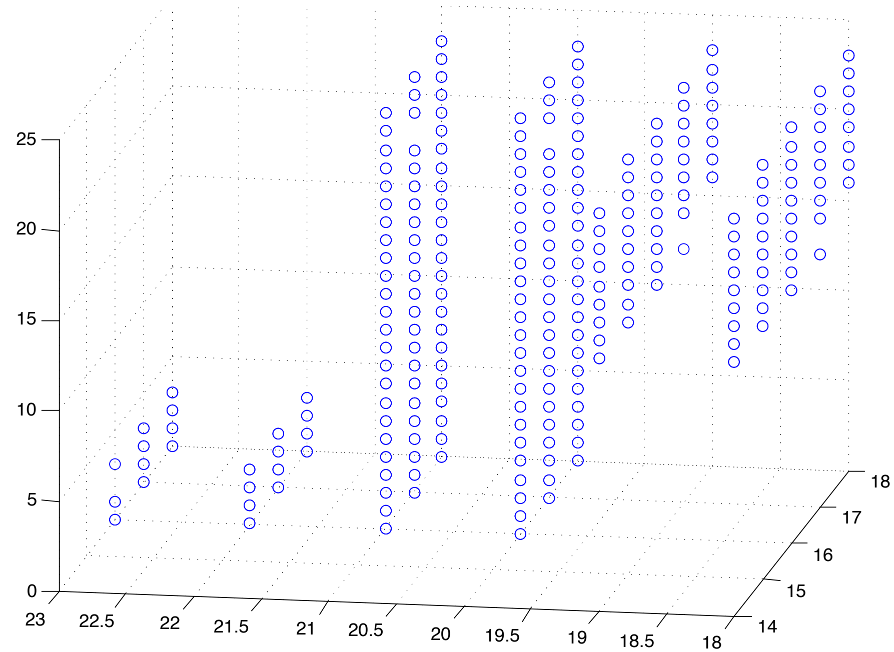
Further Graph Queries

```
MPI_Topo_test(MPI_Comm comm, int *status)
```

- Status is either:
  - MPI_GRAPH
  - MPI_CART
  - MPI_DIST_GRAPH
  - MPI_UNDEFINED (no topology)
- Enables to write libraries on top of MPI topologies!

Algorithms and Topology

- Complex hierarchy:
  - Multiple chips per node; different access to local memory and to interconnect; multiple cores per chip
  - Mesh has different bandwidths in different directions
  - Allocation of nodes may not be regular (you are unlikely to get a compact brick of nodes)
  - Some nodes have GPUs
- Most algorithms designed for simple hierarchies and ignore network issues



Recent work on general topology mapping e.g.,

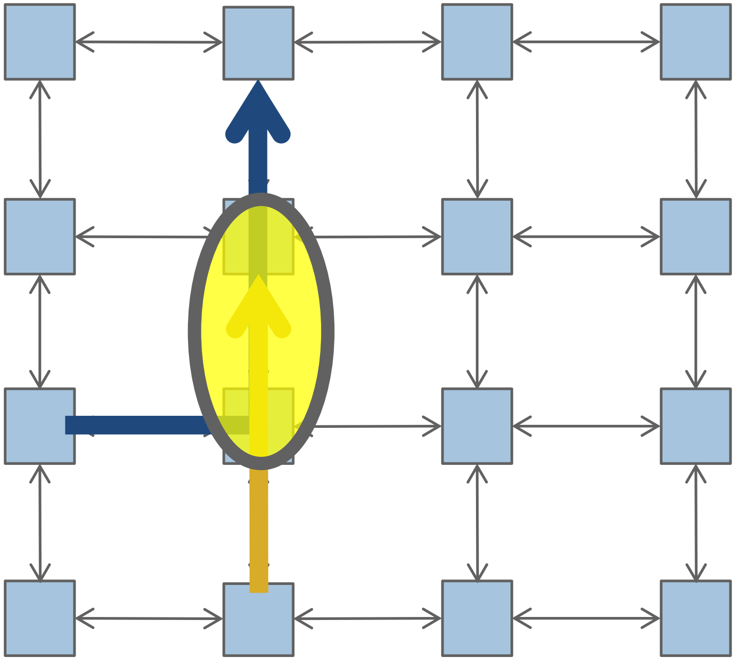
Generic Topology Mapping Strategies for Large-scale Parallel Architectures, Hoefler and Snir

Dynamic Workloads Require New, More Integrated Approaches

- Performance irregularities mean that classic approaches to decomposition are increasingly ineffective
  - Irregularities come from OS, runtime, process/thread placement, memory, heterogeneous nodes, power/clock frequency management
- Static partitioning tools can lead to persistent load imbalances
  - Mesh partitioners have incorrect cost models, no feedback mechanism
  - "Regrid when things get bad" won't work if the cost model is incorrect; also costly
- Basic building blocks must be more dynamic without introducing too much overhead

Communication Cost Includes More than Latency and Bandwidth

- Communication does not happen in isolation
- Effective bandwidth on shared link is ½ point-to-point bandwidth
- Real patterns can involve many more (integer factors)
- Loosely synchronous algorithms ensure communication cost is worst case



Halo Exchange on BG/Q and Cray XE6

- 2048 doubles to each neighbor
- Rate is MB/sec (for all tables)

BG/Q	8 Neighbors	
	Irecv/Send	Irecv/Isend
World	662	1167
Even/Odd	711	1452
1 sender		2873

Cray XE6	8 Neighbors	
	Irecv/Send	Irecv/Isend
World	352	348
Even/Odd	338	324
1 sender		5507

Discovering Performance Opportunities

- Lets look at a single process sending to its neighbors.
- Based on our performance model, we *expect* the rate to be roughly twice that for the halo (since this test is only sending, not sending and receiving)

System	4 neighbors		8 Neighbors	
		Periodic		Periodic
BG/L	488	490	389	389
BG/P	1139	1136	892	892
BG/Q			2873	
XT3	1005	1007	1053	1045
XT4	1634	1620	1773	1770
XE6			5507	

Discovering Performance Opportunities

- Ratios of a single sender to all processes sending (in rate)
- *Expect* a factor of roughly 2 (since processes must also receive)

System	4 neighbors		8 Neighbors	
		Periodic		Periodic
BG/L	2.24		2.01	
BG/P	3.8		2.2	
BG/Q			1.98	
XT3	7.5	8.1	9.08	9.41
XT4	10.7	10.7	13.0	13.7
XE6			15.6	15.9

- BG gives roughly double the halo rate. XTn and XE6 are much higher.
  - It should be possible to improve the halo exchange on the XT by scheduling the communication
  - Or improving the MPI implementation

Neighborhood Collectives

Neighborhood Collectives

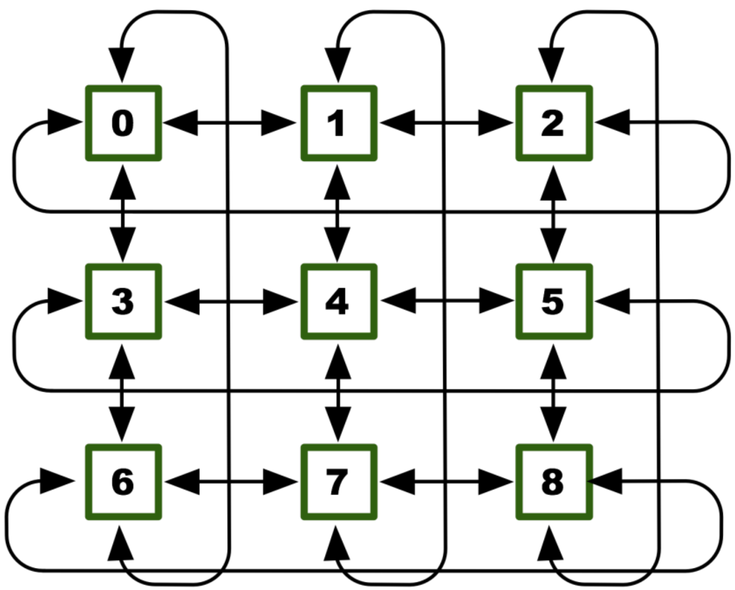
- Topologies implement no communication!
  - Just helper functions
- Collective communications only cover some patterns
  - E.g., no stencil pattern
- Several requests for “build your own collective” functionality in MPI
  - Neighborhood collectives are a simplified version
  - Cf. Datatypes for communication patterns!

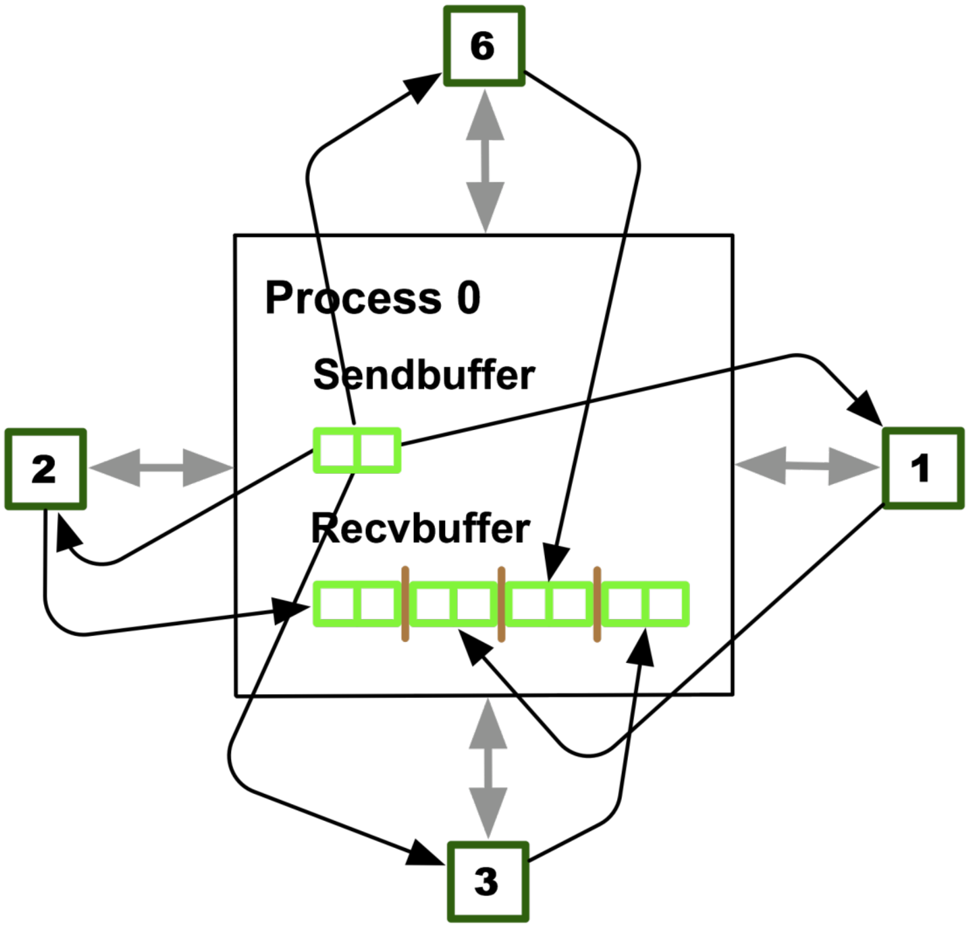
Cartesian Neighborhood Collectives

- Communicate with direct neighbors in Cartesian topology
  - Corresponds to cart_shift with disp=1
  - Collective (all processes in comm must call it, including processes without neighbors)
  - Buffers are laid out as neighbor sequence:
    - Defined by order of dimensions, first negative, then positive
    - 2*ndims sources and destinations
    - Processes at borders (MPI_PROC_NULL) leave holes in buffers (will not be updated or communicated)!

Cartesian Neighborhood Collectives

- Allgather
- Buffer ordering example:





Graph Neighborhood Collectives

- Collective Communication along arbitrary neighborhoods
  - Order is determined by order of neighbors as returned by (dist_)graph_neighbors.
  - Distributed graph is directed, may have different numbers of send/recv neighbors
  - Can express dense collective operations ☺
  - Any persistent communication pattern!

MPI_Neighbor_allgather

```
MPI_Neighbor_allgather(const void* sendbuf, int sendcount,
MPI_Datatype sendtype, void* recvbuf, int recvcount,
MPI_Datatype recvtype, MPI_Comm comm)
```

- Sends the same message to all neighbors
- Receives indegree distinct messages
- Similar to MPI_Gather
  - The all prefix expresses that each process is a “root” of his neighborhood
- Also a vector “v” version for full flexibility

MPI_Neighbor_alltoall

```
MPI_Neighbor_alltoall(const void* sendbuf, int sendcount,
MPI_Datatype sendtype, void* recvbuf, int recvcount,
MPI_Datatype recvtype, MPI_Comm comm)
```

- Sends outdegree distinct messages
- Received indegree distinct messages
- Similar to MPI_Alltoall
  - Neighborhood specifies full communication relationship
- Vector and w versions for full flexibility

Nonblocking Neighborhood Collectives

```
MPI_Ineighbor_allgather(…, MPI_Request *req);
MPI_Ineighbor_alltoall(…, MPI_Request *req);
```

- Very similar to nonblocking collectives
- Collective invocation
- Matching in-order (no tags)
  - No wild tricks with neighborhoods! In order matching per communicator!

Topology Summary

- Topology functions allow users to specify application communication patterns/topology
  - Convenience functions (e.g., Cartesian)
  - Storing neighborhood relations (Graph)
- Enables topology mapping (reorder=1)
  - Not widely implemented yet
  - May requires manual data re-distribution (according to new rank order)
- MPI does not expose information about the network topology (would be very complex)

Neighborhood Collectives Summary

- Neighborhood collectives add communication functions to process topologies
  - Collective optimization potential!
- Allgather
  - One item to all neighbors
- Alltoall
  - Personalized item to each neighbor
- High optimization potential (similar to collective operations)
  - Interface encourages use of topology mapping!

Acknowledgments

- Thanks to Torsten Hoefler and Pavan Balaji for some of the slides in this tutorial